Indian J. Phys. **76B** (5), 643–648 (2002)

I J P B
an international journal

Coherence in positron (electron) scattering by lithium atoms

P P Singh* and Sanjeev Saxena†

*Department of Physics, S R M S College of Engg & Tech., Bareilly-243 202, Uttar Pradesh, India

†Department of Physics, Bareilly College, Bareilly-243 001, Uttar Pradesh, India

E-mail : ppsingh_2000@yahoo com

Received 5 February 2002, accepted 24 May 2002

Abstract : The study of alignment and orientation parameters provides complementary information on the anisotropic charge cloud distribution (alignment) and the rotation of atomic excited state (orientation), which is not available from the measurement of differential and total cross sections alone A two potential approach is used to study these parameters in the positron (electron) impact $2s$–$3p$ excitation of lithium atom. Results are obtained for the angular variation of the angular momentum transfer ($L_\perp$), the polarization components (P_1, P_2), linear polarization (P_ℓ), polarization $|P|$ and the alignment angle (γ) at impact energies of 20 eV and 30 eV. Comparison with the corresponding parameters in electron scattering is made to see the role of various interaction potentials in the process It is found that for this transition, a significant change appears in between positron and electron impact excitation.

Keywords : Coherence, polarization, positron, electron, scattering

PACS Nos. : 34.80.Pa, 34.85 +x

1. Introduction

The discovery of positron e^+ is one of the great success of experimentalists in 20-th century physics. Positrons were observed in 1932 by Anderson in cloud chamber photographs of cosmic rays and later Blackett and Occhialini also discovered the phenomenon of pair production. Since then, the positron has become a familiar probe in the laboratory with applications stretching from fundamental physics, chemistry, condensed matter physics to medicine and engineering (positron emission tomography). Recently, interests have been focussed on positron atom (specially alkali atom) scattering. The reason of theoretical interest in alkali atoms as targets is due to its simplicity. Considerable advances have been made in our understanding of dynamics of collision processes by studying alignment and orientation parameters. The study of alignment and orientation parameters provide a great deal of information about the finer details of collision processes. The alignment is referred to the shape of the excited state charge clouds and its direction with a given quantization axis in space, while orientation gives the angular momentum transferred to atom during the course of collision which is not available from the measurement of differential cross section alone.

The dynamics of collisional excitations and the energy transfer is obtained by studying the polarization and correlation studies. The collisionally excited atom generally possesses as anisotropy in the excited state population. This anisotropy is measured by the photon angular distribution and polarization of the radiation emitted in the subsequent atomic decay. The first calculation of alignment and orientation parameters for electron lithium scattering for resonant excitation ($2s$–$2p$) was done by Saxena and Mathur [1]. For sodium resonant transition, Teubner and coworkers [2,3] have measured the spin averaged alignment and orientation parameters. McClelland *et al* [4] have reported measurement of the singlet and triplet components of the angular momentum transfer in electron-sodium resonant ($3s$–$3p$) scattering. Theoretical studies on electron-sodium scattering have been made by Purohit and Mathur [5,6] and Mitroy *et al* [7].

*Corresponding Author

As far as we know that no other theoretical results for the alignment and orientation parameters are available for the $2s$–$3p$ non-resonant transition for e^{+}-lithium atom scattering. Moreover some investigations of this process have been made by McAlinden and coworkers [8,9] using a many state close-coupling approximation without investigating the alignment and orientation parameters. They have reported the results of total cross section in the energy range 0.5 to 60 eV. It should also be mentioned that the calculations of McAlinden and coworkers [8,9] provides quite accurate representation of the coupling between various open channels. The data for coherence as well as angular momentum transfer is much useful in high temperature plasma and astrophysics. Therefore, in this paper within the frame-work of the two-potential approach we have studied the alignment and orientation parameters. Results are obtained for the angular variation of the angular momentum transfer ($L_\perp$), the polarization components (P_1, P_2), linear polarization (P_ℓ), polarization $|P|$ and the alignment angle (γ) at intermediate energies of 20 eV and 30 eV. The comparison between positron and electron scattering data on a particular target gives better insight into the scattering mechanism. Thus, comparison has also been made among the corresponding parameters.

2. Theory

The parameter λ, A^c_{1+}, O^c_1 and $L_\perp$ are related to the scattering amplitudes as given [1,10] by

$$\lambda = \frac{|a_0|^2}{|a_0|^2 + 2|a_1|^2} = \frac{\sigma_0}{\sigma_0 + 2\sigma_1},$$

$$A^c_{1+} = \sqrt{2}\,\mathrm{Re}\langle a_0 a_1\rangle/\sigma,$$

$$O^c_{1-} = -\sqrt{2}\,\mathrm{Im}\langle a_0 a_1\rangle/\sigma,$$

$$\text{and} \quad L_\perp = 2O^c_{1-} \tag{1}$$

where a_0 and a_1 are the scattering amplitudes in the collision frame for the excitation to the magnetic substates 0 and 1 respectively. σ_0 and σ_1 are the corresponding differential cross section and $\sigma = \sigma_0 + 2\sigma_1$ is the total differential cross-section summed over all magnetic substates. $L_\perp$ denotes the angular momentum transferred perpendicular to the scattering plane and < > denotes the spin averaged value of the amplitude.

In the coherence (polarization) experiments, one measures the components of the polarization of the radiation (P_1, P_2 and P_3) emitted normal to the scattering plane and expressed by

$$\begin{aligned} P_1 &= [I(0°) - I(90°)]/[I(0°) + I(90°)],\\ P_2 &= [I(45°) - I(135°)]/[I(45°) + I(135°)],\\ P_3 &= [I(\mathrm{RHC}) - I(\mathrm{LHC})]/[I(\mathrm{RHC}) + I(\mathrm{LHC})], \end{aligned} \tag{2}$$

where $I(\alpha)$ is the number of coincidence counts *i.e.* intensity when the optic axis of the polarizer is at $\alpha°$ to the incident beam direction and light is observed in a direction perpendicular to the axis. I(RHC) and I(LHC) are right and left circular polarization components respectively.

Further, the polarization components are related to the parameters of correlation experiment by Andersen *et al* [11]

$$\begin{aligned} P_1 &= 2\lambda - 1,\\ P_2 &= -2A^c_{1+},\\ P_3 &= -2O^c_{1-} = -L_\perp. \end{aligned} \tag{3}$$

The coherence of the excitation is defined by the total polarization P given by

$$|P| = \left[|P_1|^2 + |P_2|^2 + |P_3|^2\right]^{1/2}, \tag{4}$$

$$|P| = 1 \text{ implies coherent excitation.}$$

The linear polarization component (P_ℓ) which gives the normalised difference between the length and width of the charge cloud, is given by

$$P_\ell = \left(P_1^2 + P_2^2\right)^{1/2}. \tag{5}$$

The alignment angle (γ) of the charge cloud with respect to the incident beam direction is given by

$$\gamma = 0.5 \arg(P_1 + iP_2). \tag{6}$$

Assuming the lithium atom to be a one electron system with a core, the scattering amplitude for the excitation of magnetic sublevel m in the frame work of two potential approach [1] is given by

$$a^c_{M_L} = -(2\pi)^{-1}\Big[\big\langle \phi_f(r_1,r_2)|U_i|\chi_i^+(r_1,r_2) + \chi_f^-(r_1,r_2)|W_f|A\psi_i^+(r_1,r_2)\big\rangle\Big], \tag{7}$$

where the scattering particle wavefunctions satisfy the Schrödinger equation :

$$\begin{aligned} (H_0 - E)\phi(r_1,r_2) &= 0,\\ (H_0 + U_i - E)\chi_i^+(r_1,r_2) &= 0,\\ (H_0 + U_f - E)\chi_i^-(r_1,r_2) &= 0,\\ (H - E)\psi_i^+(r_1,r_2) &= 0. \end{aligned} \tag{8}$$

H is the total Hamiltonian and H_0 is the unperturbed Hamiltonian, r_1 and r_2 are the coordinates of the atomic and incident electrons respectively. A is the antisymmetrization operator.

In the two potential approach, the total interaction potential V is divided as

$$V = U_i + W_i \quad \text{in the initial channel,}$$

$$\text{and} \quad V = U_f + W_f \quad \text{in the final channel.} \tag{9}$$

If the distorting potential U_j in the channel j is chosen to depend on the incident particle coordinates only, the first term of the eq. (7) will vanish for inelastic scattering. In the distorted wave approximation (to the first order), one takes $\psi_i^+ \approx \chi_i^+$,

$$a_{M_L}^c = -(2\pi)^{-1}\left\langle \chi_f^-(r_1,r_2)\middle|W_f\middle|A\chi_i^+(r_1,r_2)\right\rangle$$

$$= f_{M_L}^c \pm g_{M_L}^c, \tag{10}$$

where $f_{M_L}^c = -(2\pi)^{-1}\left\langle \chi_f^-(r_1,r_2)\middle|W_f\middle|\chi_i^+(r_1,r_2)\right\rangle$

and $g_{M_L}^c = -(2\pi)^{-1}\left\langle \chi_f^-(r_1,r_2)\middle|W_f\middle|\chi_i^+(r_2,r_1)\right\rangle.$

In case of electron scattering, both direct ($f_{M_L}^c$) and exchange ($g_{M_L}^c$) scattering amplitudes contribute to $a_{M_L}^c$ whereas due to absence of exchange, only direct ($f_{M_L}^c$) scattering amplitude contributes in case of positron scattering.

The distorting potential U_j in the channel j is expressed as

$$U_j = V_s^j + V_c^j + V_p^j,$$

where V_s^j, V_c^j and V_p^j are the static, core and non adiabatic polarization potentials respectively as used by Saxena and Mathur [1], Thirumalai *et al* [12], Stone [13] and Walters [14]

$$V_s^j = \left\langle v_i(r_1)\middle|V\middle|v_j(r_1)\right\rangle,$$

$$V_c^i = -2(1/r_2 + 2.7)\exp(-5.4r_2),$$

$$V_c^f = -2(1/r_2 + 1/2\mu)\exp(-r_2/\mu) \tag{11}$$

with $\mu = 0.301939$ for Li

and $V_p^j = \left\langle v_j(r_1)\middle|V\middle|v_j^{\text{pol}}(r_1,r_2)\right\rangle \chi_p^j(r_2),$

where the perturbed wavefunctions $v_j^{\text{pol}}(r_1,r_2)$ are obtained following the procedure of Stone [13]. For s and p states, they are written as

$$v_{ns}^{\text{pol}}(r_1,r_2) = \beta_{ns}(r_2)\sum_m Y_{\ell m}^*(\hat{r}_2)v_{npm}(r_1), \text{ for } s \text{ states.}$$

$$\text{and} \quad v_{npm}^{\text{pol}}(r_1,r_2) = \beta_{np}(r_2)Y_{\ell m}(\hat{r}_2)v_{ns}(r_1), \quad \text{for } p \text{ states.}$$

The function $\beta_j(r_2)$ are obtained by solving the pair of equations

$$\left\langle v_{ns}(r_1)\middle|H_A + V - E\middle|\left(v_j(r_1) + v_j^{\text{pol}}(r_1,r_2)\right)\right\rangle = 0,$$

$$\left\langle v_{npm}(r_1)\middle|H_A + V - E\middle|\left(v_j(r_1) + v_j^{\text{pol}}(r_1,r_2)\right)\right\rangle = 0,$$

where H_A is the atomic Hamiltonian. Analytical wavefunctions [13–15] are used in obtaining the above potentials.

If one consideres only the adiabatic polarization, then the factor $\chi_p^j(r_2)$ in eq. (10) is taken to be unity. This will be the case at low energies. However, at intermediate energies non-adiabatic effects would become important and to account for the same, we express $\chi_p^j(r_2)$ as [12]

$$\chi_p^j(r_2) = \frac{1}{\left(1 + 6k_j^2/\omega^2 r_2^2\right)}, \tag{12}$$

k_j is the scattered electron momentum and ω is the average excitation energy.

3. Results and discussion

In this section, we present our results for positron and electron scattering of Li ($2s$–$3p$) excitation for energies 20 eV and 30 eV. We have calculated the coherence parameters (P_1, P_2, P_3), linear polarization (P_ℓ), polarization $|P|$, alignment angle (γ) and angular momentum transferred perpendicular to scattering plane $L_\perp$ for this transition of lithium atom.

Figure 1 shows the angular variation of P_1, P_2 and P_ℓ at 20 eV for both electron and positron scattering. It is observed that in lower angular region *i.e.* below 30°, there is rapid and smooth decrease in P_1 for positron impact except a hump at about 6°. After 30°, the variation is quite smooth moving from negative region to positive unity. But in case of electron

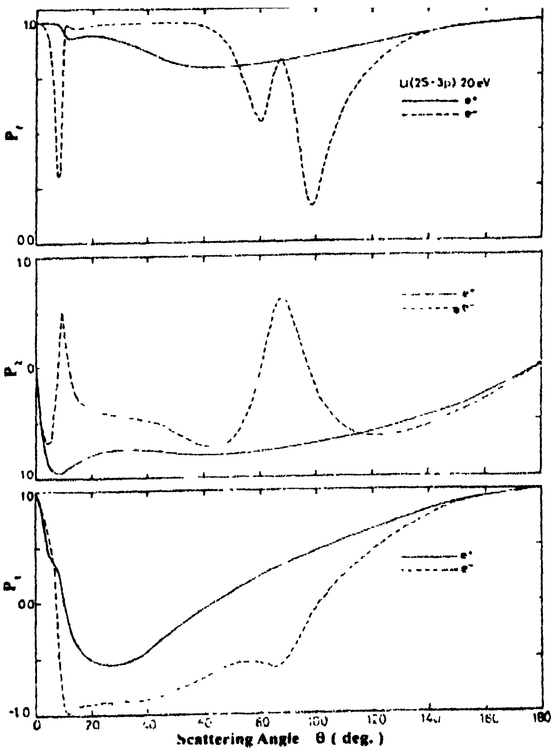

Figure 1. Polarization parameters P_1, P_2 and P_ℓ for the $2s$–$3p$ excitation of lithium at an incident energy of 20 eV
——— Present results for positron impact,
. . . . results for electron impact

impact, P_1 shows much rapid decrease in lower angular region (< 10°) and their after increase further except a dip at about 85°. In case of P_2 for positron impact, a dip is observed at 10°. However for electron impact P_2, we observed two dips and two peaks in angular region 4° to 10° and 60° to 90°. The variation of P_ℓ for positron impact shows the decrease of P_ℓ in lower angular region and after it there is a continuous increase in whole angular region, while for electron impact P_ℓ, there are three dips at 10°, 80° and 100°. From Figure 1 we also observe that variation of P_1, P_2 and P_ℓ are quite smooth for positron impact specially in higher angular region with small dips in lower angular region. But in case of electron impact, the dips and peaks are observed in angular region 5° to 100°. This behaviour confirms the role of exchange contribution in lower angular region.

In Figure 2, the angular variation of angular momentum transfer $L_\perp$ and alignment parameter γ is plotted at 20 eV incident energy. We notice that positron $L_\perp$ remains negative in almost whole angular region except below 8° and its variation is quite smooth in whole angular region except to a dip at about 10°. In case of electron $L_\perp$, we find that it is positive in the low angle region with a maximum at about 10°. While remaining close to zero between 15°–80° scattering angles, the angular momentum transfer acquires negative value with increase in angles. On acquiring a maximum negative (a dip) value, $L_\perp$ changes its sign between 80°–100°. For scattering angles beyond 100°, the $L_\perp$ decreases slowly and remains positive. This behaviour of $L_\perp$ is in contrast to the $2s$–$2p$ excitation of lithium atom as discussed by Mathur and coworkers [5,6] where $L_\perp$ remains positive for low and intermediate angles and negative for higher angles. The negative value of γ for positron case signifies that charge cloud is aligned away from the scattered positron.

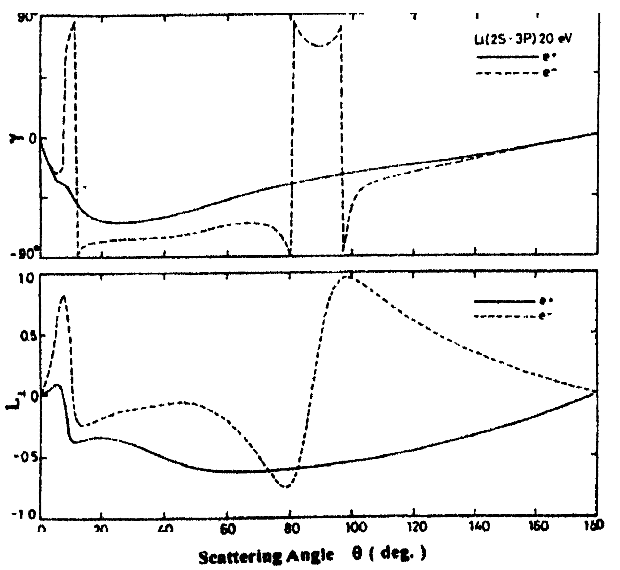

Figure 2. $L_\perp$ and γ for $2s$–$3p$ excitation of lithium at an incident energy of 20 eV. Full and broken curves denote the same as in Figure 1.

But for electron impact, the charge cloud is aligned towards the incident particle, as it posses positive value at low angles beyond which it is aligned away from the incident particle (negative value of γ).

Figures 3 and 4 show the angular variation of (P_1, P_2, P_ℓ) and ($L_\perp$, γ) respectively at 30 eV incident energy.

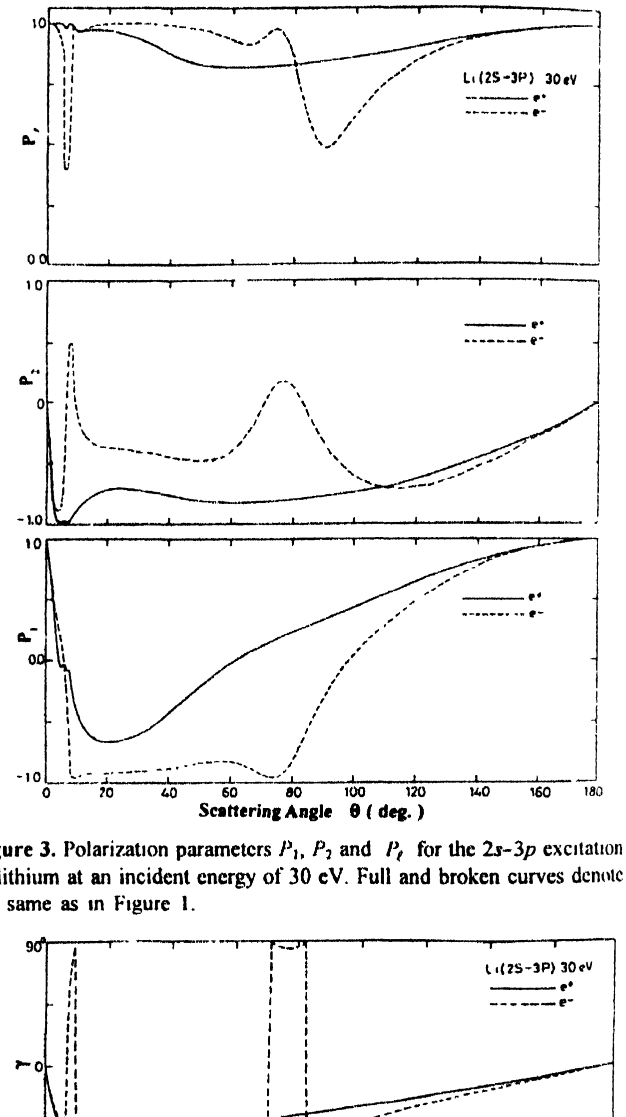

Figure 3. Polarization parameters P_1, P_2 and P_ℓ for the $2s$–$3p$ excitation of lithium at an incident energy of 30 eV. Full and broken curves denote the same as in Figure 1.

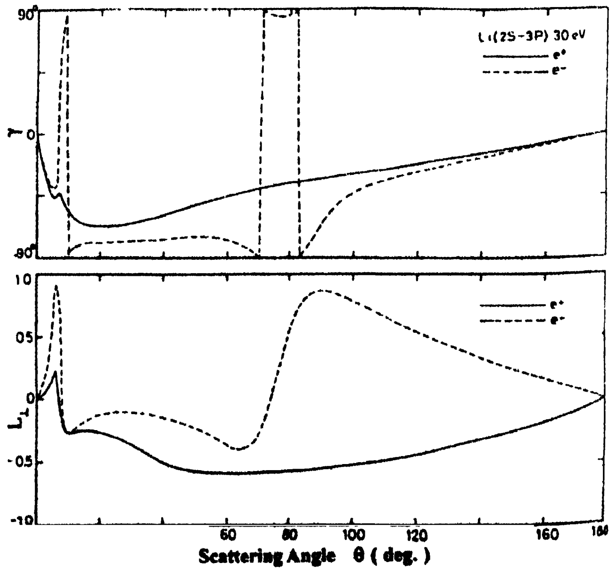

Figure 4. $L_\perp$ and γ for $2s$–$3p$ excitation of lithium at an incident energy of 30 eV. Full and broken curves denote the same as in Figure 2

The general features of these results at this energy are similar to that as 20 eV with a shift of dips and peaks towards lower scattering angles as discussed earlier.

Table 1 shows the angular variation of polarization $|P|$. We find that except for angles between 80°–100° at 20 eV and 2° and 8° at 30 eV, the $2s$–$3p$ excitation of lithium by electron impact is nearly coherent. This loss of coherence at certain scattering angles results from the magnitude of exchange contribution at these angles. For the excitation of a doublet p state, the exchange effect leads to different amplitudes for singlet and triplet scattering. The density matrix involves an incoherent average over the singlet and triplet scattering amplitudes which gives rise to incoherence. At a particular scattering angle, the exchange contribution would depend on the overlap of the incident electron wavefunction and the atomic electron wavefunction. Hence, for those scattering at which this overlap is large, there would be a significant deviation for the values of $|P|$ from unity (perfect coherence). However, in case of positron, impact variation of $|P|$ is unity in entire angular rang. It confirms complete coherence of excitation process in positron case.

Table 1. Polarization $|P|$ for the electron and positron impact excitation ($2s$–$3p$) of lithium at 20 eV and 30 eV energies

Energy →	20 eV		30 eV	
Angle (degree)	Electron	Positron	Electron	Positron
0	1.0	1.0	1.0	1.0
2	1.0	1.0	0.90	0.97
4	1.0	1.0	1.0	1.0
6	1.0	1.0	0.98	1.0
8	0.98	1.0	0.90	1.0
10	1.0	1.0	1.0	1.0
20	0.98	1.0	1.0	0.98
30	0.99	1.0	1.0	1.00
40	1.0	1.0	0.99	0.99
50	1.0	1.0	0.99	0.99
60	1.0	1.0	0.99	0.96
70	1.0	1.0	1.0	0.99
80	0.97	1.0	1.0	0.99
90	0.94	1.0	1.0	0.99
100	0.98	1.0	1.0	1.0
110	1.0	1.0	1.0	0.99
120	1.0	1.0	1.0	1.0
130	1.0	1.0	0.99	1.0
140	1.0	1.0	1.0	1.0
150	1.0	1.0	0.99	1.0
160	1.0	1.0	1.0	1.0
170	1.0	1.0	0.98	0.99
180	1.0	1.0	1.0	1.0

4. Conclusions

From the above study, we conclude that as impact energy increases, the magnitude of first peak appearing at about 5°, also increases indicating the equal contribution of singlet and triplet scattering channels. This feature may be easily observed for all parameters. Also the behavior of coherence for $2s$–$3p$ excitation differs significantly from $2s$–$2p$ excitation due to non resonant and resonant transitions. At present, no other theoretical as well as experimental data are available to compare with present calculations. We except the data to become available soon in near future as experimental studies with lithium atoms are in progress at Beilefeld University by Baum and collaborators in Germany. We hope that present study would stimulate more work in this field.

It should be mentioned that McAlinden *et al* [8] reported the variation of total cross section with energy (range 0.5–60 eV) for positron scattering by lithium. These authors have not reported the results of differential cross section. On the other hand, we have reported the angular variation of coherence parameters which requires the variation of differential cross section with scattering angle at a particular energy. Thus, the present calculations differ from those presented by McAlinden *et al* [8]. However, such theoretical efforts are very important for researchers engaged in experimental work.

Acknowledgments

Authors are thankful to the referee for his comments which helped us in revising the manuscript. We wish to express our sincere gratitude, for necessary infrastructure provided to us by the Principal, Bareilly College, Bareilly. One of us (PPS) thanks to Shri Dev Murti, Chairman, SRMS College of Engg. & Tech., Bareilly, for encouragement and providing excellent computing facilities for the above work. We are highly indebted to Dr. M Kumar for his advice on present work.

References

[1] S Saxena and K C Mathur *J Phys* **B18** 509 (1985)

[2] P J O Teubner, J L Riley, M J Brunger and S J Buckman *J. Phys.* **B19** 3313 (1986)

[3] M J Brunger, J L Reiley and P J O Teubner *J. Phys* **B22** 655 (1989)

[4] J J McClelland, M H Kelley and R J Celotta *Phys. Rev.* **A40** 2321 (1989)

[5] S P Purohit and K C Mathur *J. Phys* **B23** L473 (1990)

[6] K C Mathur and S P Purohit *J. Phys.* **B22** L223 (1989)

[7] J Mitroy, I E McCarthy and A T Stelbovics *J. Phys.* **B20** 4827 (1987)

[8] M T McAlinden, A A Kernoghan and H R J Walters *J. Phys.* **B30** 1543 (1997)

[9] H R J Walters, A A Kernoghan, M T McAlinden and C P Campbell *Pramana* **50** 573 (1998)

[10] M Eminyan, K MacAdam, J Slevin and H Kleinpoppen *J. Phys.* **B7** 1519 (1974); *Phys. Rev. Lett.* **31** 576 (1973)

[11] N Andersen, J W Gallagher and I V Hertel *Phys. Rep* **165** 1 (1988)

[12] D Thirumalai, D G Truhlar, M A Brandt, R A Eades and D A Dixon *Phys. Rev.* **A25** 2946 (1982)

[13] P M Stone *Phys. Rev.* **141** 137 (1966)

[14] H R J Walters *J. Phys.* **B6** 1003 (1973)

[15] D Rapp and C M Chang *J. Chem. Phys.* **57** 4283 (1972)